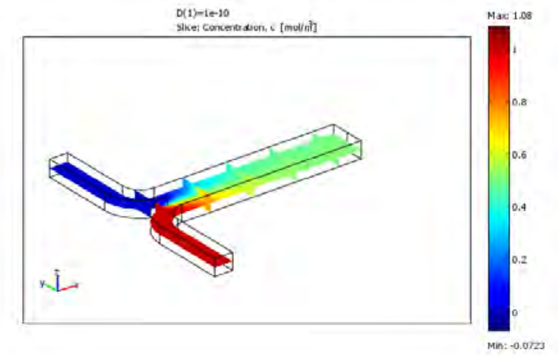
COMSOL Conference 2008 Boston
Fourth Annual Conference on Multiphysics Simulation

Renaissance Boston Waterfront
October 9-11, 2008 Boston, MA

Development of an Interlinked Curriculum Module for Microchemical Process System Components Using COMSOL Multiphysics

Session on *Numerical Methods & Education* - October 10, 2008



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ChE Curriculum Reform Project
- Objectives -

Provide ChE students with the knowledge to:

- Apply fundamental ideas over an expanded range of time and length scales.
- Apply ChE fundamental ideas to emerging application areas.
- Construct solutions for more complex, more open-ended synthesis tasks.
- Transfer fundamentals and knowledge to novel challenges.

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Scope of Implementation

- Curriculum Content Reform & Development
  - Course Strings*
  - Interlinked Curriculum Components ⬅
  - Service Learning
- Student Assessment and Evaluation
- Faculty Development

*http://www.che.tamu.edu/curriculum-reform/course-strings

Interlinked Curriculum Components (ICCs)

- An **ICC** is a web-based resource for teaching and learning
- ICC's could be used at many different points in the 4-year ChE curriculum
- ICC's will focus on:
  - Introducing new content not covered elsewhere
  - Reinforcing concepts and fundamentals
  - Demonstrating conservation principles to emerging technologies (nano, bio, energy..)

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ICC Components and Topic Coverage

- 5 principal parts
  - Pre-test
  - Topic notes
  - Examples
  - Exercises
  - Post-test
- Conservation & Continuum Principles
- Materials
- Molecular simulation
- Nanotechnology
- Microprocess systems
- Nanotechnology
- Environment and Sustainability

http://che.tamu.edu/orgs/NSFCR/

Microprocess Systems ICC

Objectives:

1. Introduce MEMS as applied to microreaction systems
2. Broaden exposure to multi-scale analysis
3. Strengthen understanding & insight into system behavior

Focus Areas:

• **MEMS & microreactors**	**Components, materials, & fabrication processes**
• **Microfluidics**	**Fluid mechanics at the microscale**
• **Transport phenomena**	**Coupled momentum & energy transport**
• **Transport-kinetic Interactions**	**Coupled momentum, energy, & species transport**
• **Device & system design**	**Microprocess component & system performance**

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Microchemical System ICC Modules

- **Module I**: Fundamentals used for modeling fluid mechanics, heat and mass transfer in microsystems.

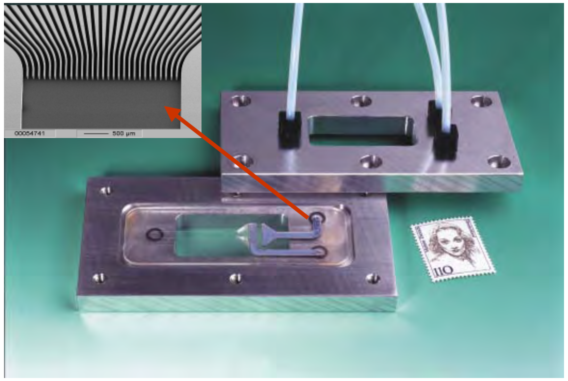
- **Module II**: Development of micro-component simulations and steady-state performance analysis.

- **Module III**: Expanding steady-state analysis to transient and multi-scale analysis along with process control elements

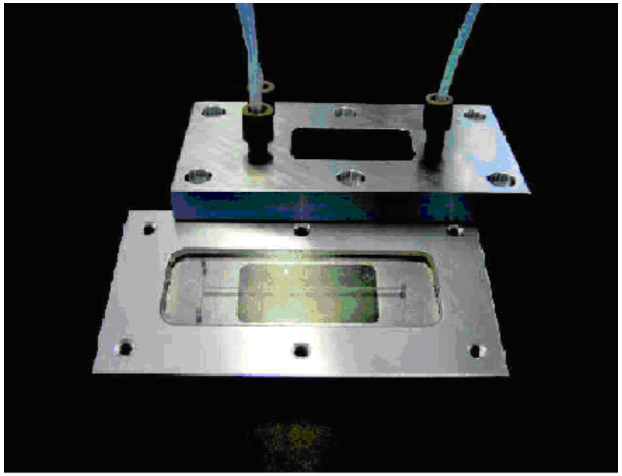
- **Module IV**: Simulation of an entire microsystem process by interfacing the various microsystem process components developed in previous modules.

Some Examples of Microprocess System Components

Falling Film Gas-liquid Microreactor



Interdigitial Micromixer for Two-phase Systems



Tee-Micromixer (Glass)

Cross-flow Heat Exchanger

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Examples of Module Problems

Microfluidics

- 2-D transient flow in a rectangular channel
- 3-D transient flow in a rectangular channel

Coupled Momentum & Energy Transport

- 2-D steady-state non-isothermal flow in a laminate structure.
- 2-D non-isothermal flow in Si rectangular channel with a Pt laminate heater.

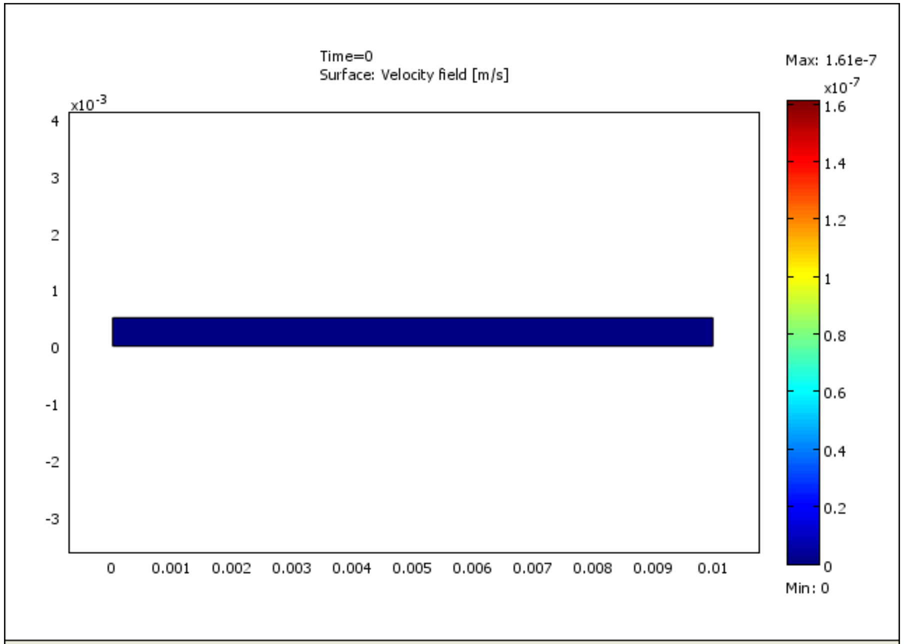
Momentum & Species Transport

- 2-D diffusion example with varying flux.
- 3-D steady-state fluid mixing in a tee-micromixer

2-D Transient Flow in a Rectangular Channel

Model Parameters

- Size: 10 mm x 0.5 mm
- Pressure drop : 0.05 Pa



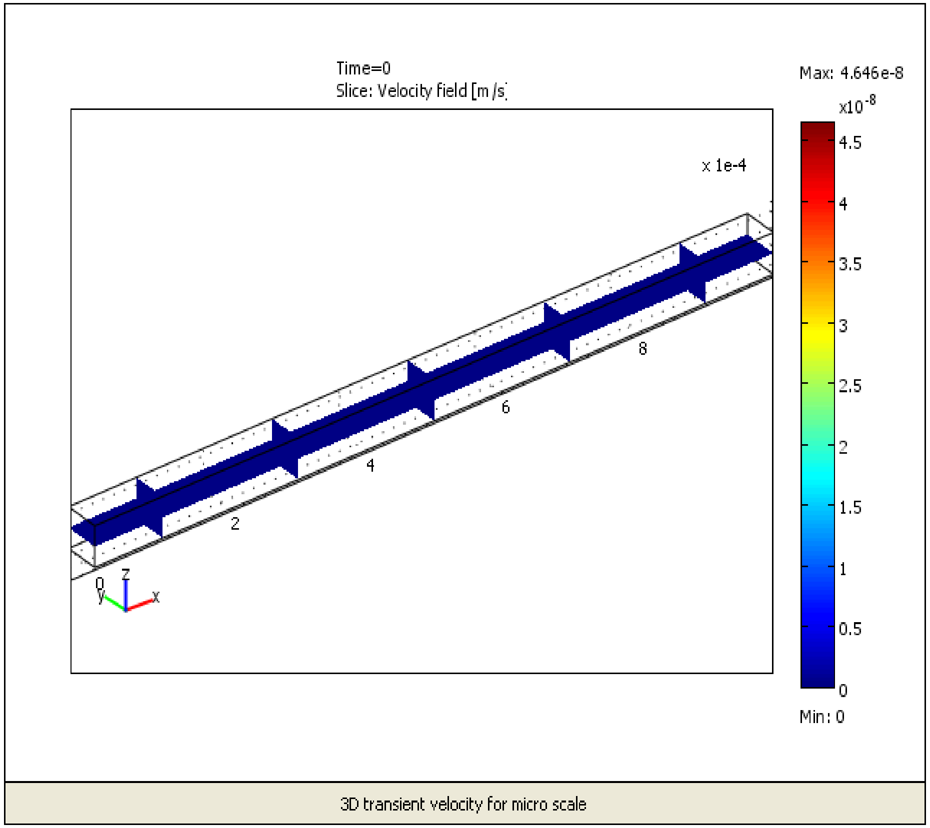
2D transient velocity for micro scale

3-D Transient Flow in a Duct

- Extension of the 2-D model
- 3-D Transient velocity profiles

Model Parameters

- Size: 10 mm x 0.5 mm
- Pressure drop : 0.05 Pa



3D transient velocity for micro scale

Effect of Re on Entrance Length in a Microchannel – Definition

- **Objective:** Study the developing transient velocity profile and entrance length effect with varying Re.

- **Key Assumptions**
  - Newtonian, Incompressible fluid
  - No external forces other than pressure difference
  - No frictional losses

- **Model Equations**
  - **Dimensionless Navier-Stokes equations**

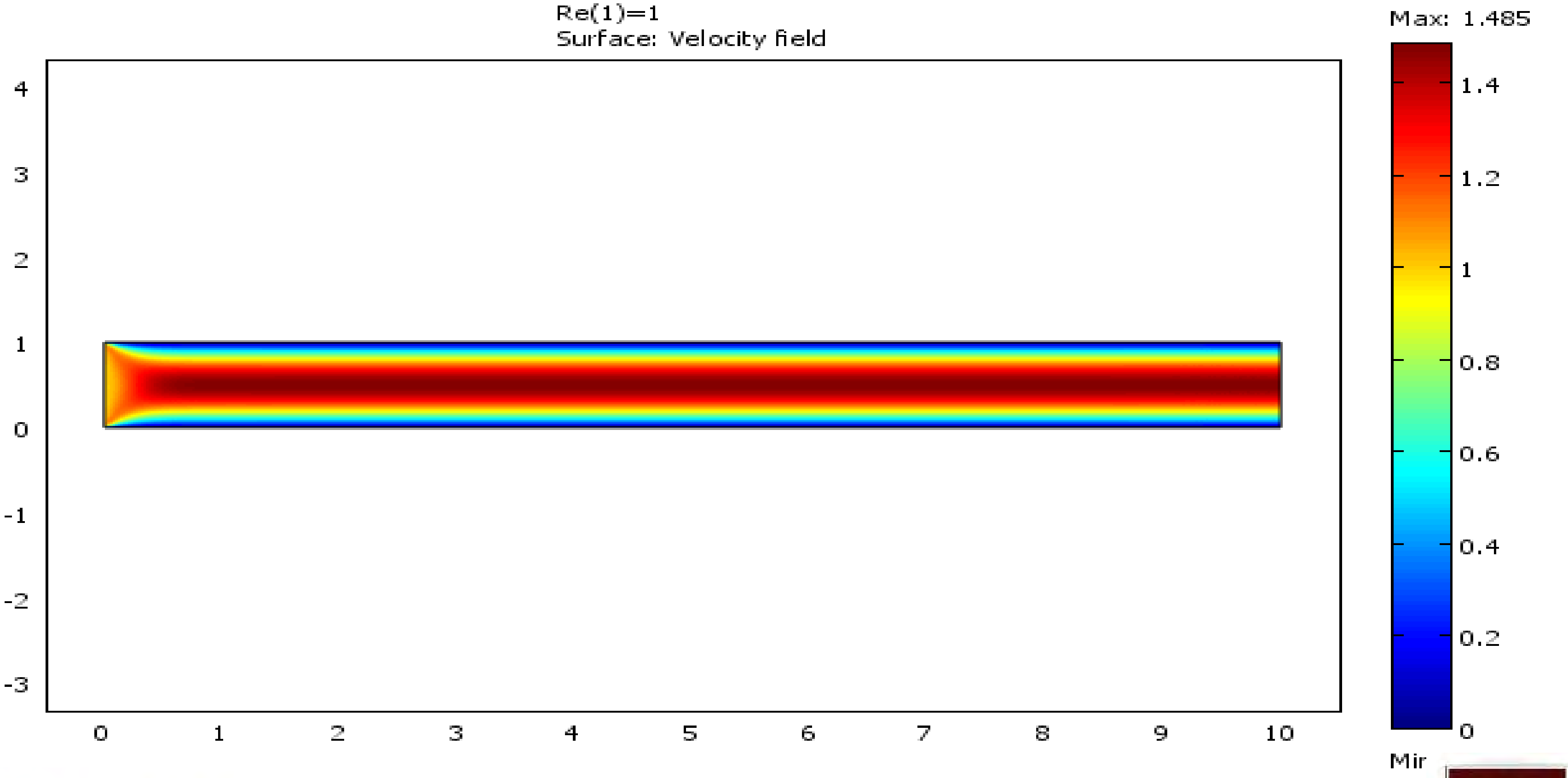
$$\frac{\partial u^*}{\partial t^*} + (u^* \bullet \nabla) u^* + \nabla p^* = \nabla \bullet \frac{1}{Re} (\nabla u^* + (\nabla u^*)^T) + F^*$$

$$\nabla \bullet u^* = 0$$

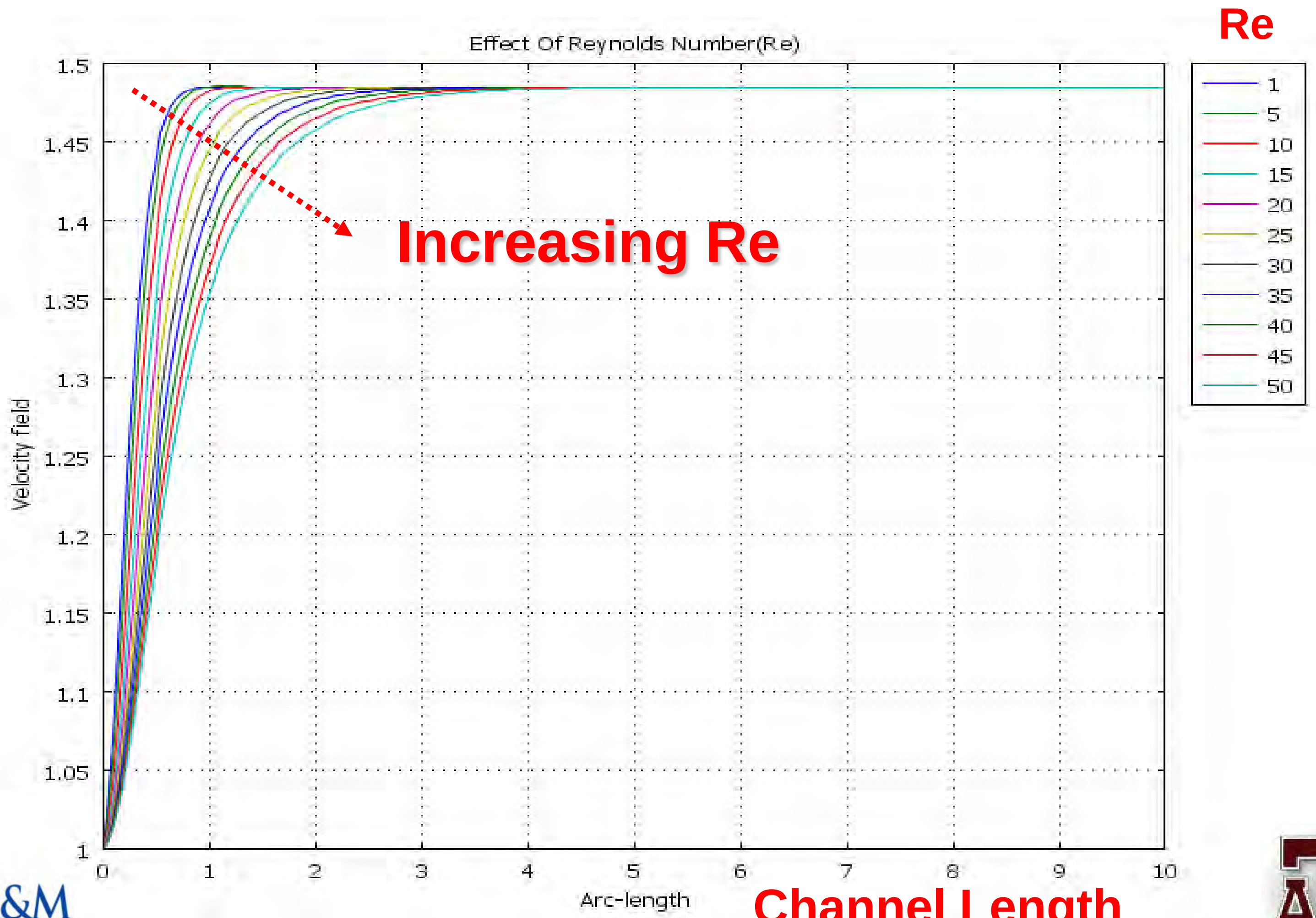
where: $u^* = u / U$ $t^* = t\, U / L$, L being an appropriate length scale,

$p^* = p / (\rho U^2)$ $F^* = F\, L / (\rho\, U^2)$

Effect of Re on Entrance Length in a Microchannel - Simulation



Effect of Re on Entrance Length in a Microchannel – Parametric Study



Channel Length

Analytical vs Simulated Entry Length

- Analytical formula to calculate the entry length in micro-processes calculated by Atkinson *et al.* using the FEM

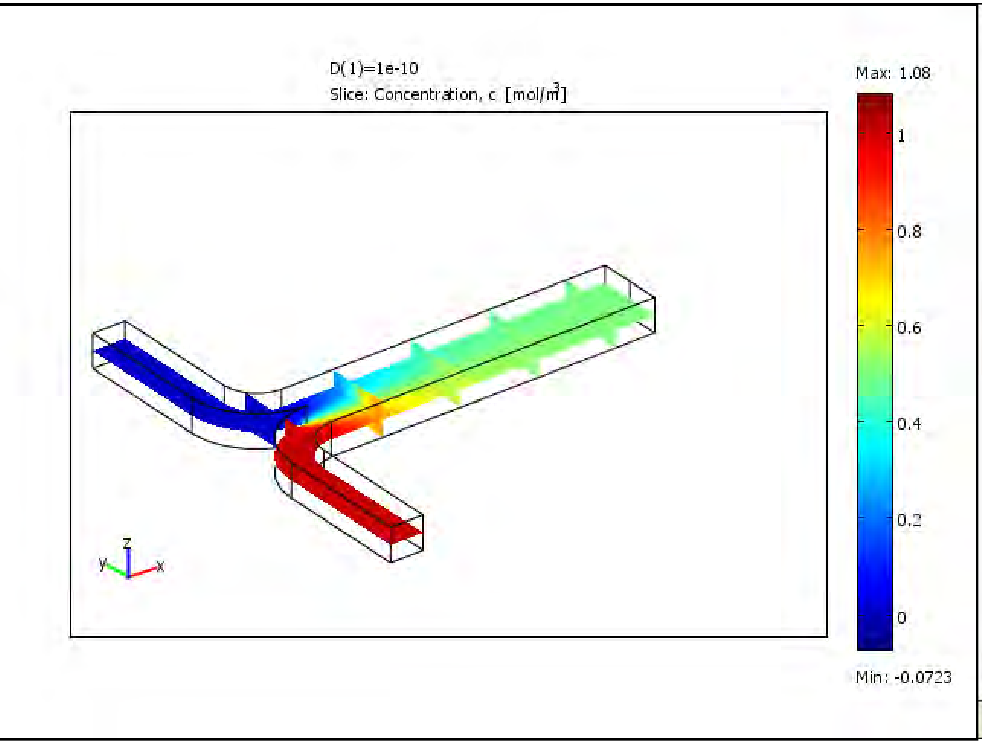
$$\frac{\mathbf{Le}}{\mathbf{D}} = \mathbf{0.59 + 0.056\,Re}$$

Le = Entrance length

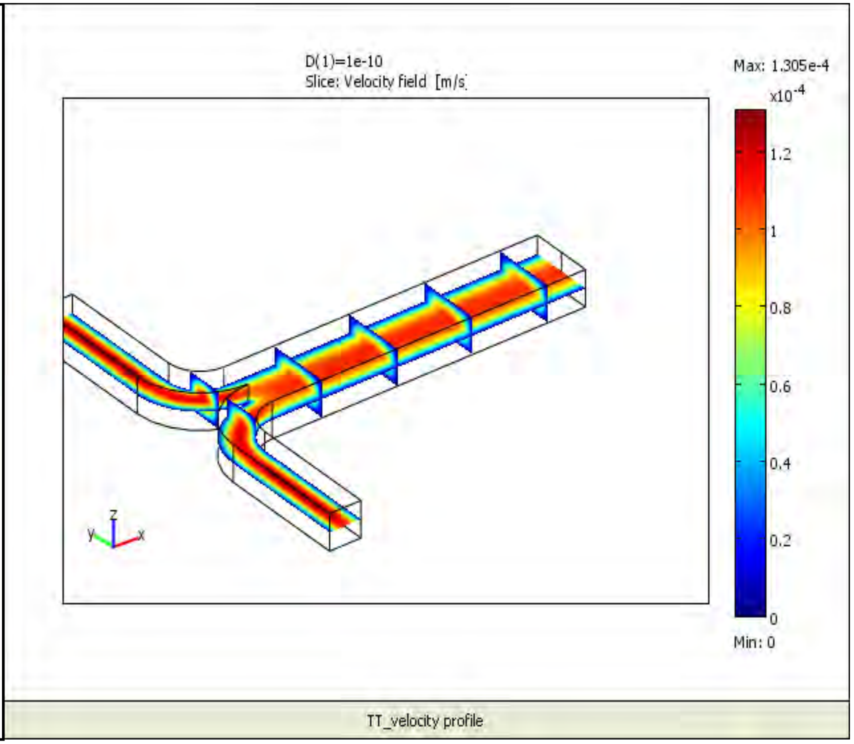
D = Pipe diameter or channel height

Re	**(Formula)*10^{-3}**	**(Simulated)*10^{-3}**
1	0.646	0.7
5	0.87	0.75
10	1.15	1
15	1.43	1.3
20	1.71	1.6
25	1.99	1.8
30	2.27	2.1
35	2.55	2.4
40	2.83	2.8
45	3.11	3
50	3.39	3.2

3-D Steady State Fluid Mixing in a Tee Micromixer - Simulations



Concentration Profile



Velocity Profile

Tee Micromixer: Mixing Effectiveness and Assessment of Mixing Quality

- **Mixing Effectiveness**

  $\tau = T_v / T_D = D\,L / v\,h^2$ where $T_v = L/v$

  $T_D = h^2/D$

  τ can be used to make predictions for mixing effectiveness

  - A low τ means fluid moves faster along the channel length compared to transverse diffusion.

- **Measure of Mixing**

  - For a simple 2D case, the measure of mixing is defined as

Measure of Mixing =

$$1-\left\{\int_0^h \frac{(c(y)-{}^{c0}\!/_{2})}{Li.c0}\,dy\right\}$$

where: c= concentration,

Li= size of the inlet of the mixing channel,

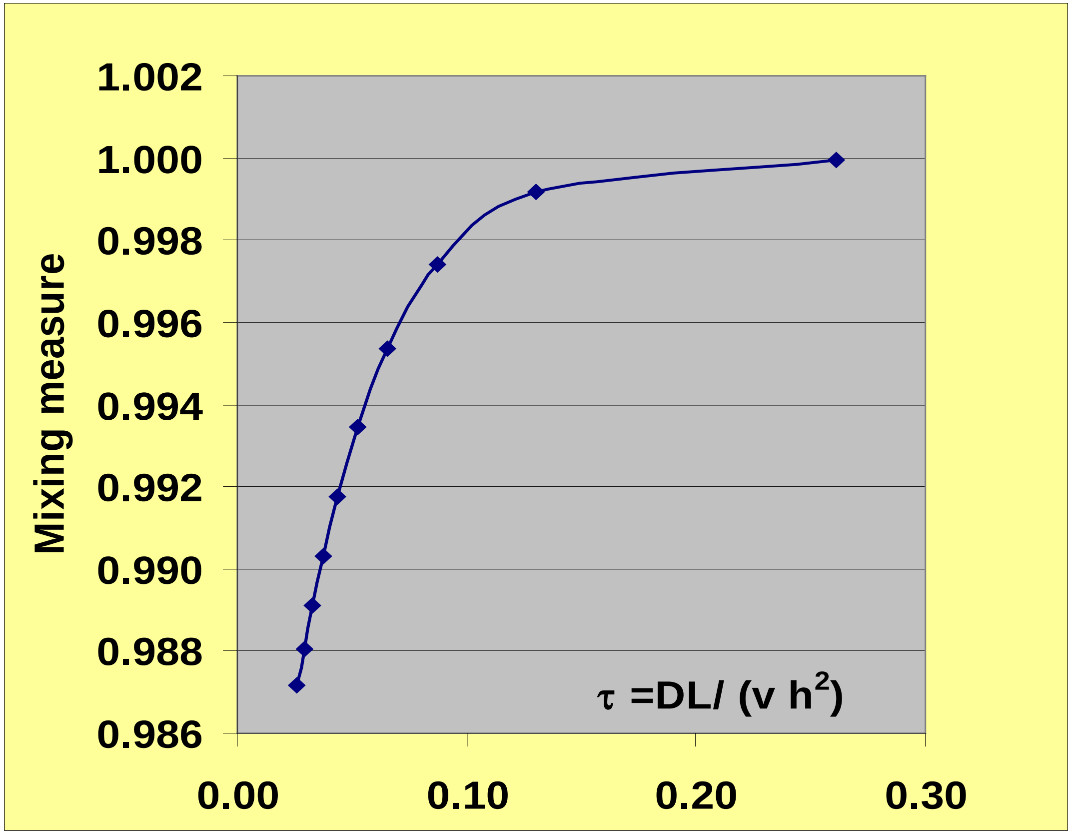
c_0= initial concentration for the mixing channel

Measure of Mixing = 1 Perfect mixing

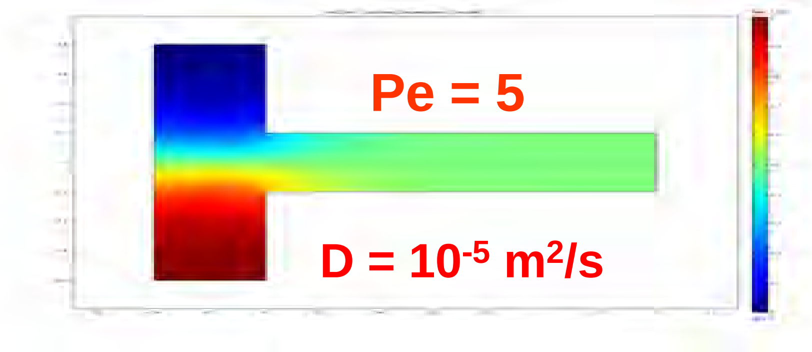
Measure of Mixing = 0 No mixing

Tee Micromixer: Effect of τ on the Measure of Mixing

- Vary τ by varying the fluid inlet velocity
- Evaluate mixing effectiveness and the measure of mixing

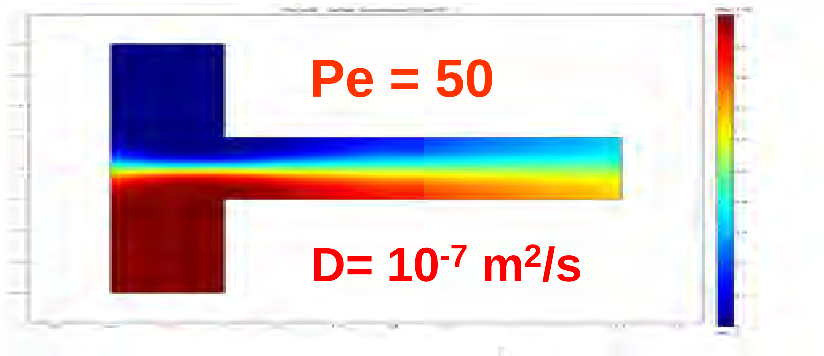


Tee Micromixer: Effect of Peclet Number on Mixing Quality



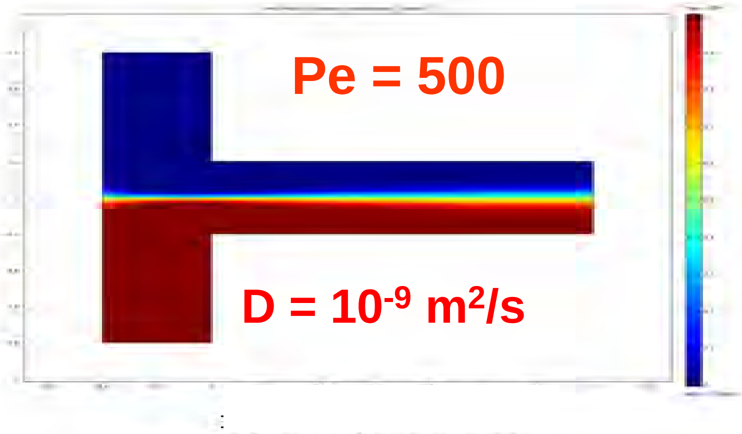
$Pe = 5$

$D = 10^{-5}\ m^2/s$



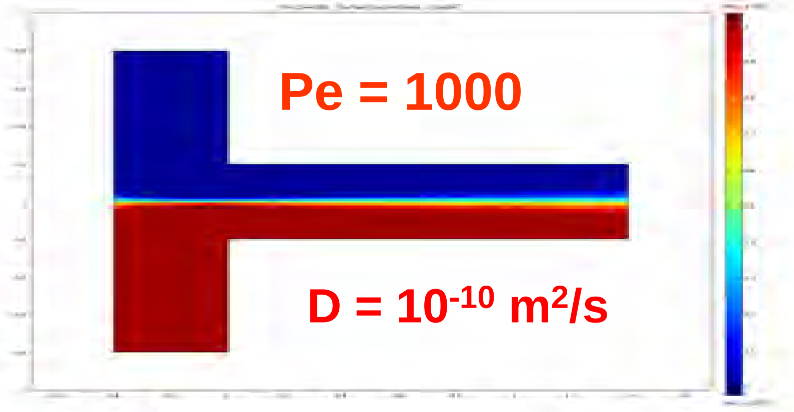
$Pe = 50$

$D = 10^{-7}\ m^2/s$



$Pe = 500$

$D = 10^{-9}\ m^2/s$

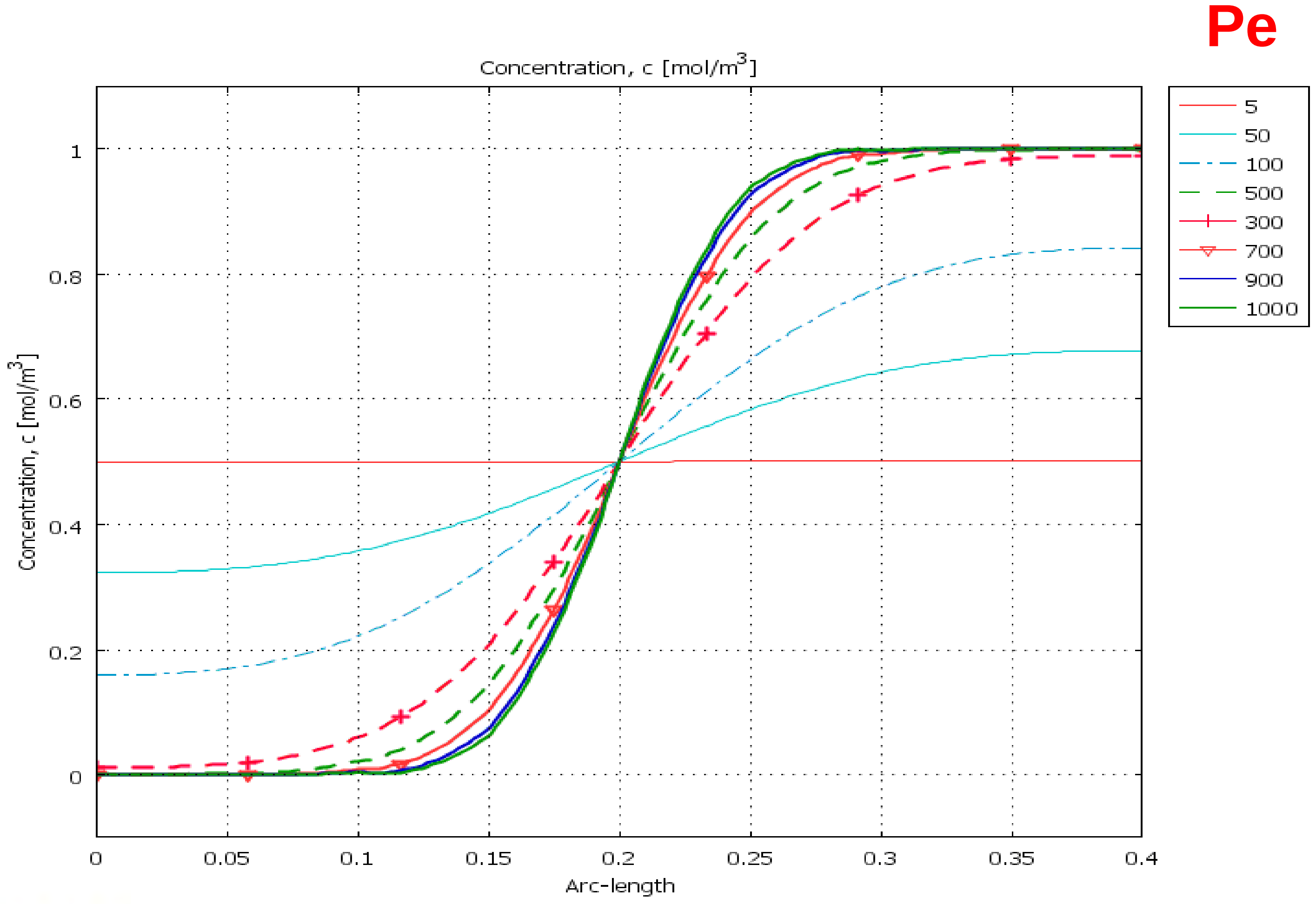


$Pe = 1000$

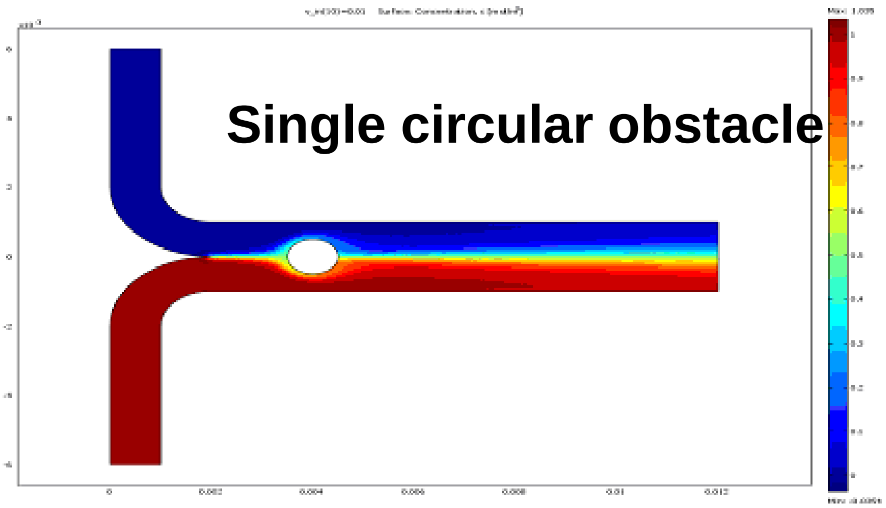
$D = 10^{-10}\ m^2/s$

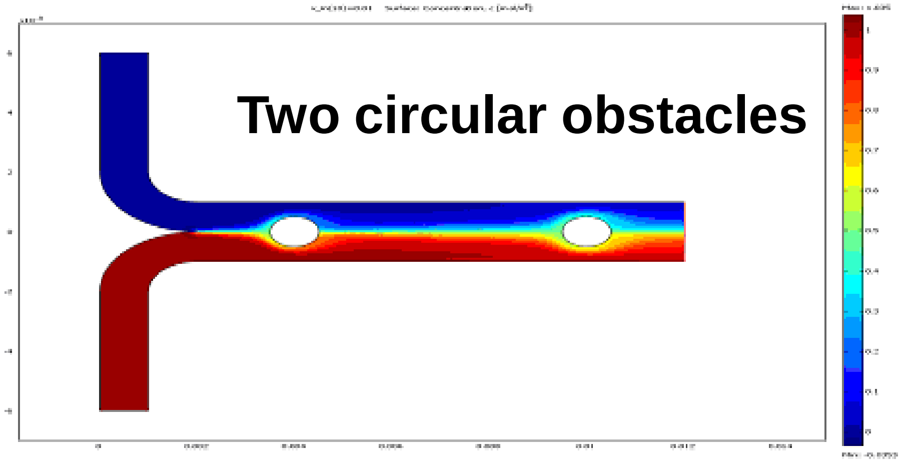
$Pe = u L / D = (L^2/D) / (L/u)$ = Diffusion time / Transport time

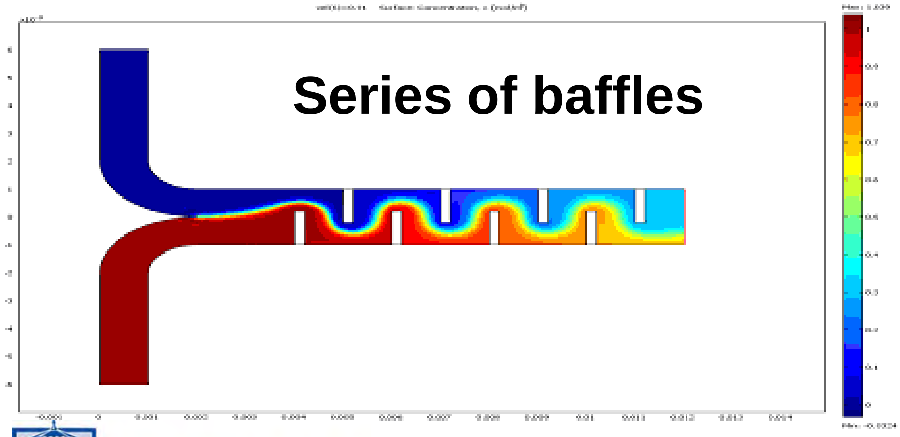
Solute Concentration Profiles vs Pe



Tee Micromixer with Different Obstacles - Concentration Profiles


Single circular obstacle


Two circular obstacles


Series of baffles

Objective

To examine the effect of different obstacles & varying velocities on mixing quality

Tee Micromixer with Different Obstacles - Simulations

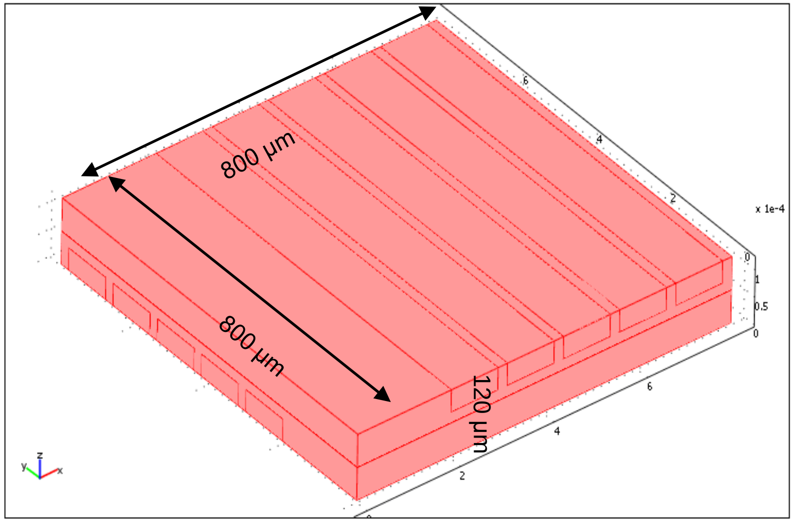
Effect of Fluid Velocity on the Measure of Mixing

Velocity	Measure of Mixing			
m/s	No obstacle	One circular obstacle	Two circular Obstacles	Baffled obstacles
0.005	0.9672	0.96612	0.9987	0.9987
0.007	0.9515	0.9505	0.952727	0.9946
0.008	0.9454	0.944424	0.9468	0.991576
0.009	0.94027	0.93925	0.941725	0.988
0.01	0.9358	0.9348	0.9373	0.984142

- **Students can readily quantify the effects of various system parameters**

Micro-scale Heat Exchanger

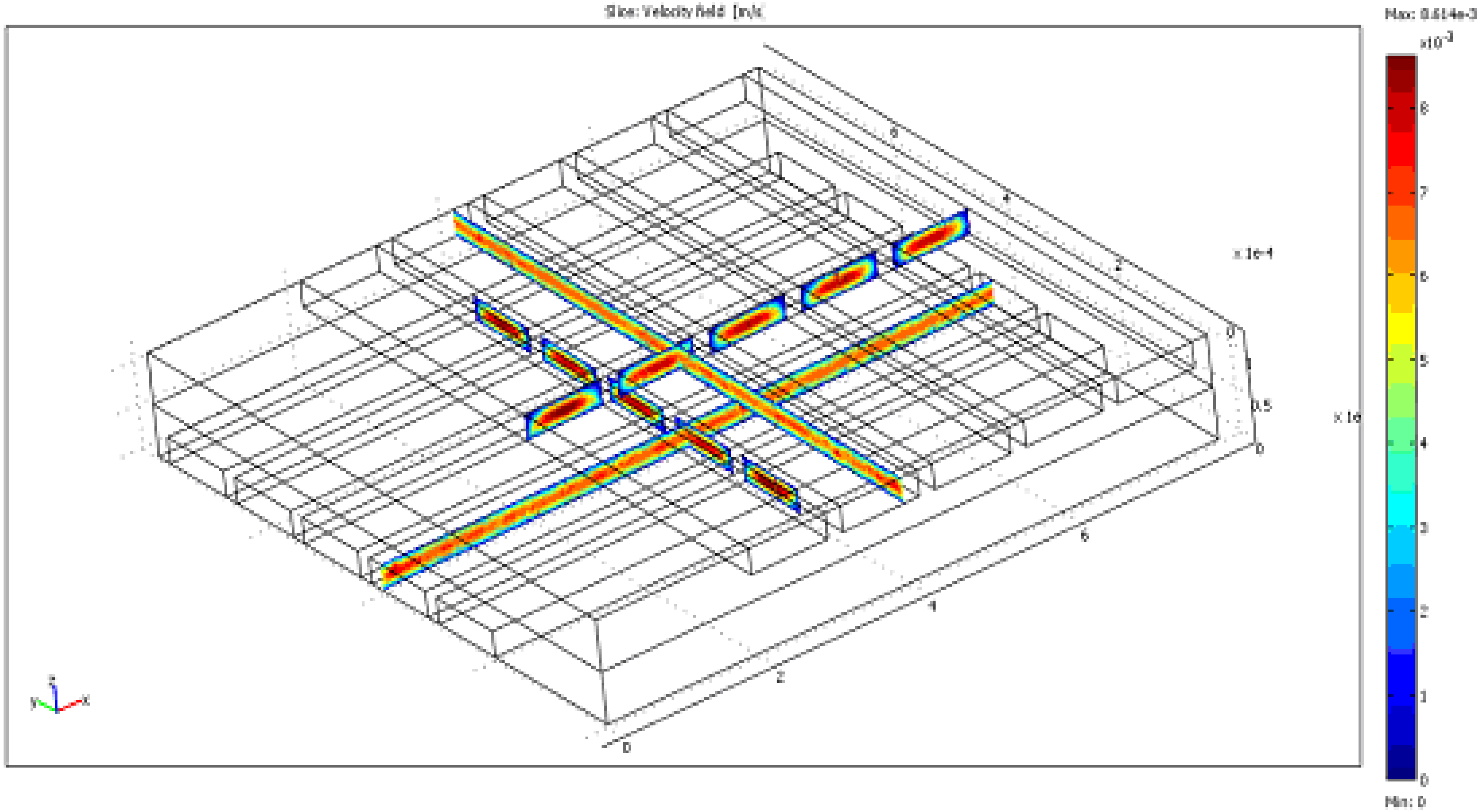
- **Objective**
  - Compare the heat exchanger effectiveness factor for various aspect ratios and fluid contacting patterns
  - Demonstrate solutions for the conduction-convection equation for a 3-D geometry
- **Model Geometry**



- **Dimensions**

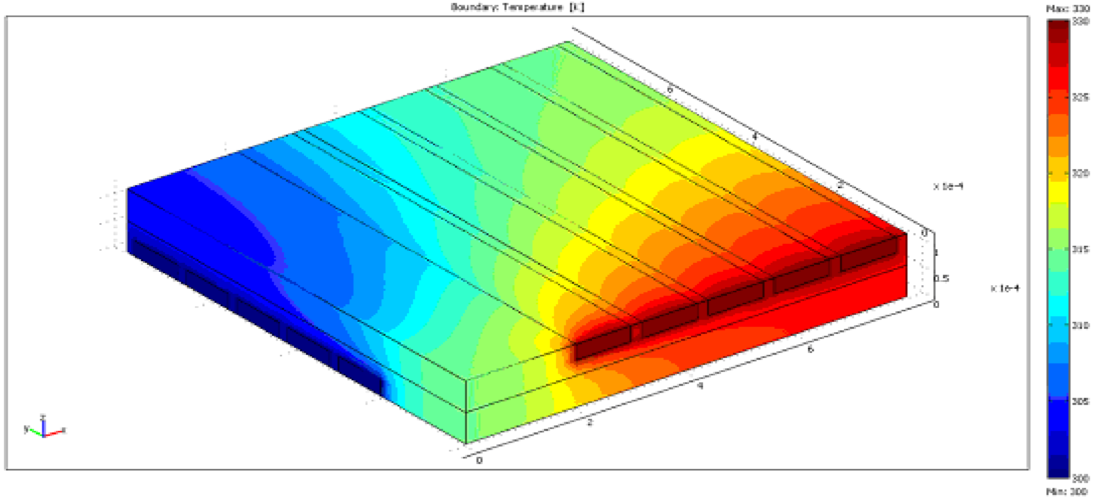
– Length of each slab	800 µm
– Width of each slab	800 µm
– Height of each slab	60 µm
– No. of Microchannels	5
– Microchannel width	100 µm
– Microchannel height	30 µm
– Mat'l of Construction	Steel

Velocity Profiles

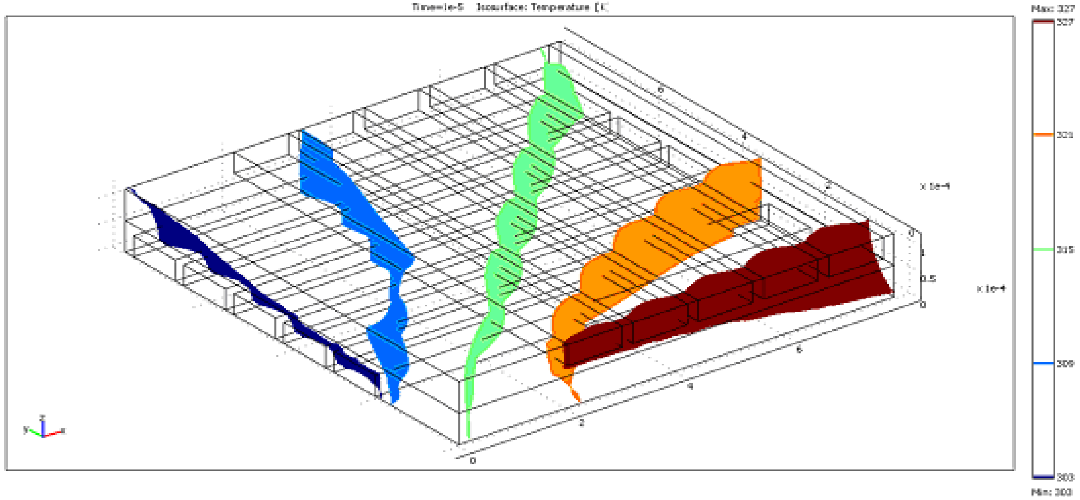


Temperature Profiles

Surface Plot



Isosurface Plot



Micro-Heat Exchanger Effectiveness Based on Aspect Ratio

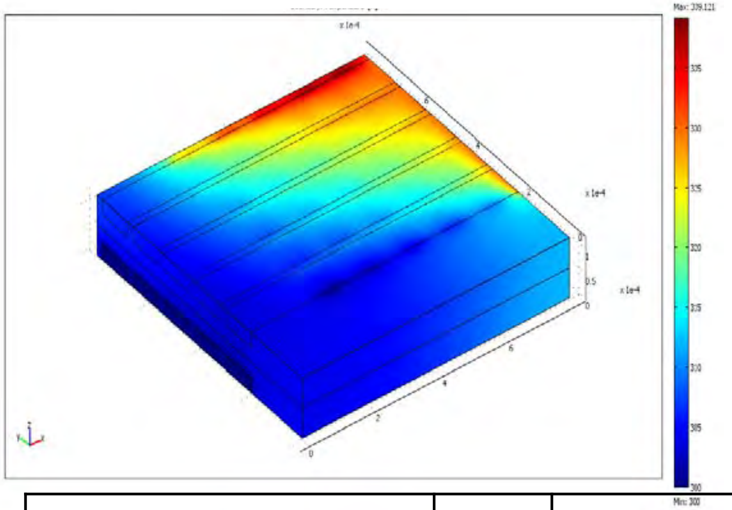
- The aspect ratio (h/w) of the 3-D MEMS heat exchanger is varied by altering the height (h) of the microchannel
- Effectiveness Factor $\varepsilon = \frac{Q}{Q_{max}} = \frac{m\,C_p\,(T_{hot,\,in} - T_{hot,\,out})}{m\,C_p\,(T_{hot,\,in} - T_{cold,\,in})}$

h, μm	w, μm	Aspect Ratio	$T_{h,out}$ K	$T_{c,out}$ K	Effectiveness Factor
30	100	0.3	**312.17**	**317**	**0.5943**
40	100	0.4	**311.73**	**318.23**	**0.6090**
50	100	0.5	**311.39**	**318**	**0.6203**

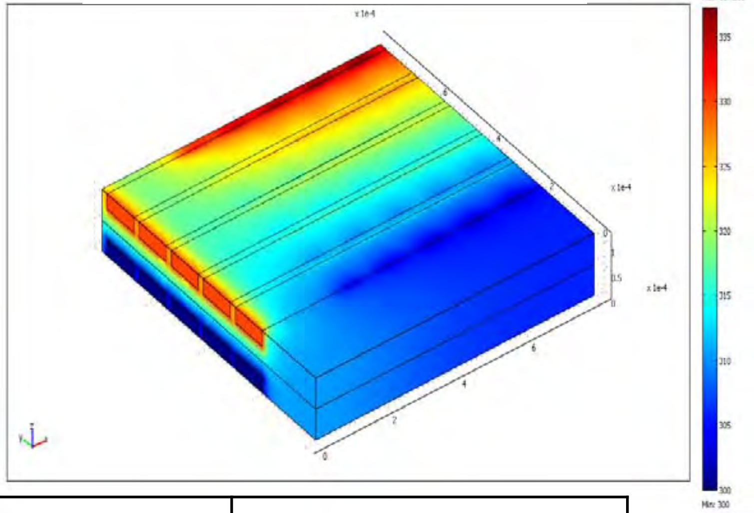
Comparing Cocurrent, Countercurrent and Cross Flow

- Compare the effectiveness factor for various contacting modes

Countercurrent flow



Cocurrent flow

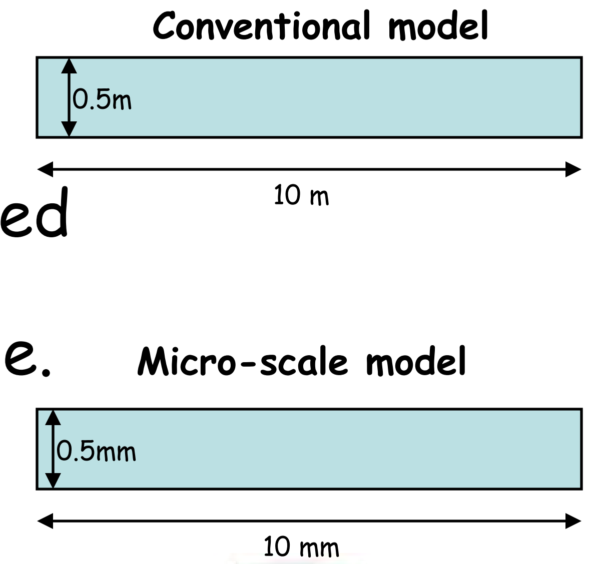


Contacting	**h**	**$T_{out,h}$**	**$T_{out,c}$**	**Effectiveness**
Mode	**μm**	**K**	**K**	**η**
Cross-flow	30	312.17	317	0.5943
Countercurrent	30	304.62	325.19	0.8460
Cocurrent	30	318.19	318.18	0.3937

2-D Steady-State Non-isothermal Flow in a Laminate Structure

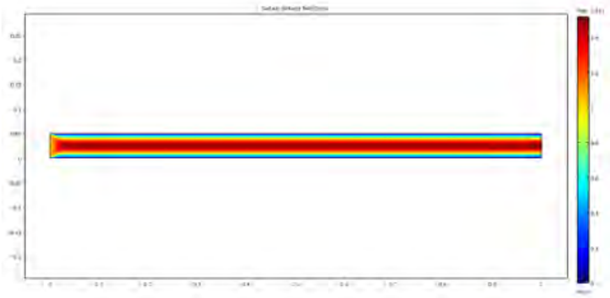
- A non-isothermal temperature profile is obtained for a fluid flowing through a rectangular laminate along with a laminar velocity profile.

- The velocity and temperature profiles obtained for the micro scale are compared with those obtained from a conventional scale model with the same residence time.

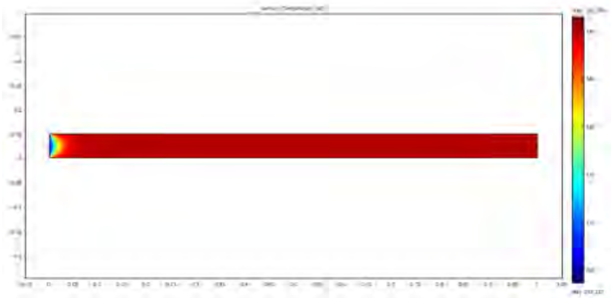


2-D Steady-State Non-isothermal Flow in a Laminate Structure

Conventional Model

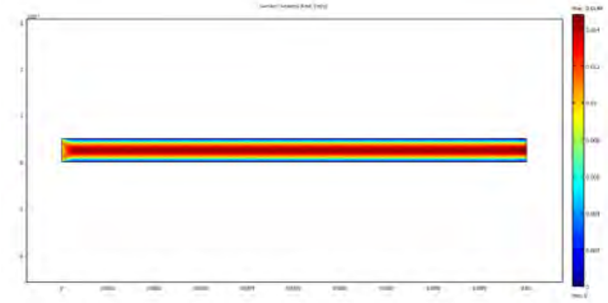


Velocity Profile

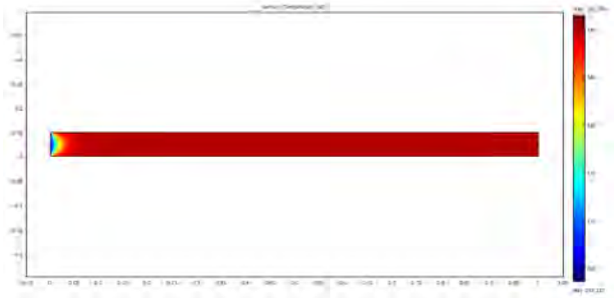


Temperature Profile

Micro-scale Model



Velocity Profile



Temperature Profile

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2-D Steady-State Non-isothermal Flow in a Laminate Structure

Comparison of Results

Parameter	Conventional Model	Micro-scale Model
Mean Residence Time	1 s	1 s
Maximum Velocity, m/s	1.511	0.0151
Maximum Temperature, K	352.78	352.78

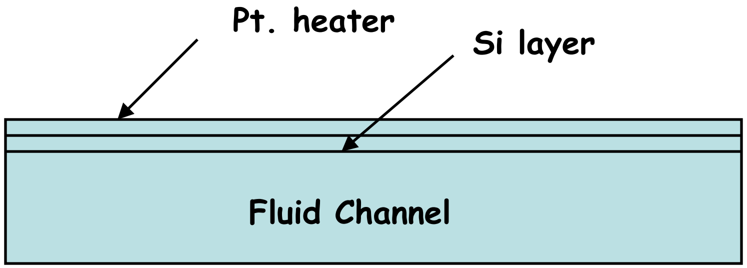
2-D Non-isothermal Flow in a Si Microchannel with Wall-Catalyzed Reaction

- Mass, energy and momentum equations are coupled to find the temperature & concentration profiles for a wall-catalyzed reaction involving a dilute solute

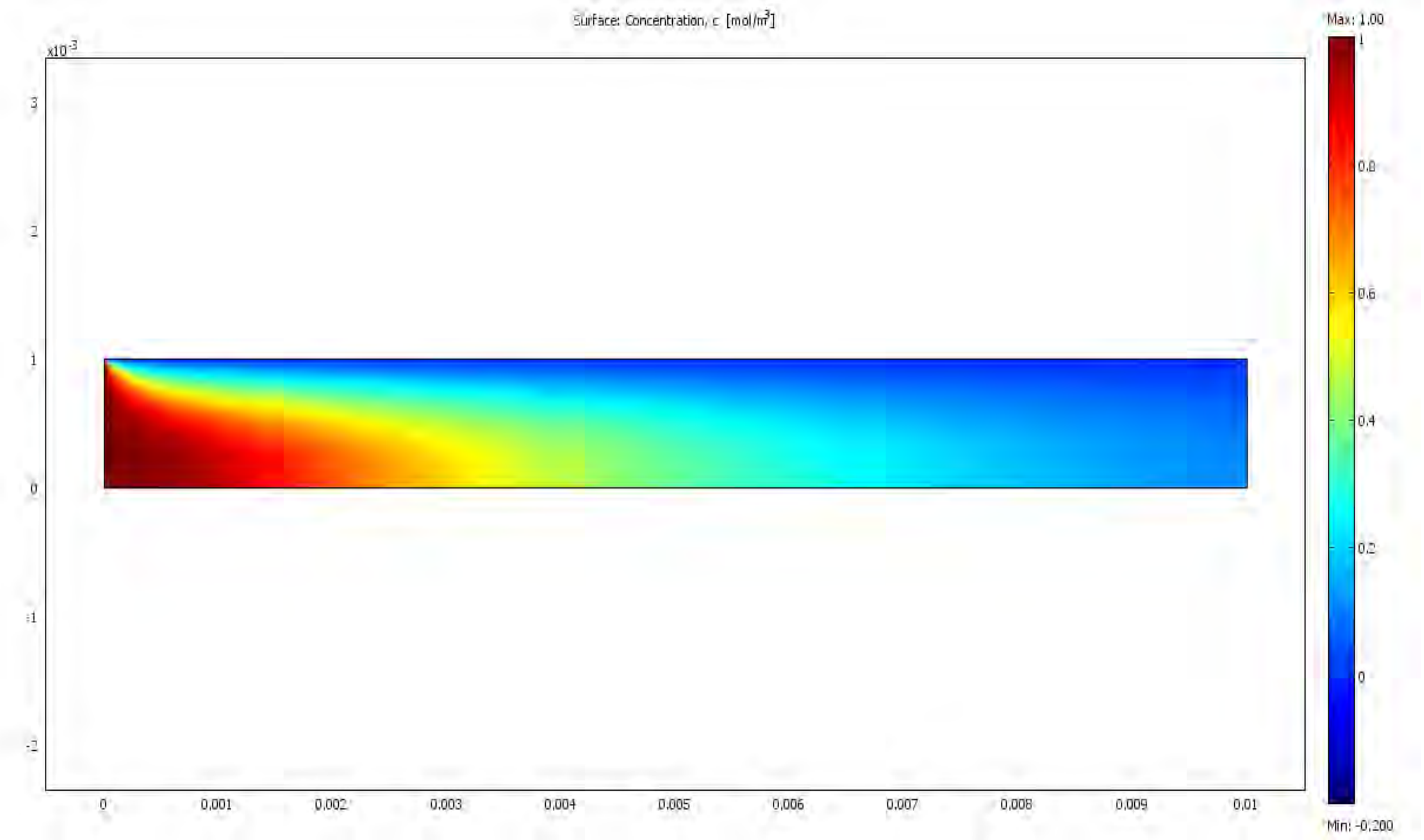
- Multi-laminate structure with Pt-Si layer on top of the channel.

- Model Dimensions

Pt heater:	20 mm x 0.1 mm
Si layer:	20 mm x 0.1 mm
Fluid channel:	20 mm x 0.6 mm



Concentration Profiles



Homogenous Gas Phase Tee Microreactor

- Single Gas-phase Homogeneous Reaction $a\,A + b\,B \rightarrow c\,C + d\,D$

$r_1 = k_f\, C_A^{\,n}\, C_B^{\,m}$

$$r_1 = -\frac{r_A}{a} = -\frac{r_B}{b} = \frac{r_C}{c} = \frac{r_D}{d}$$

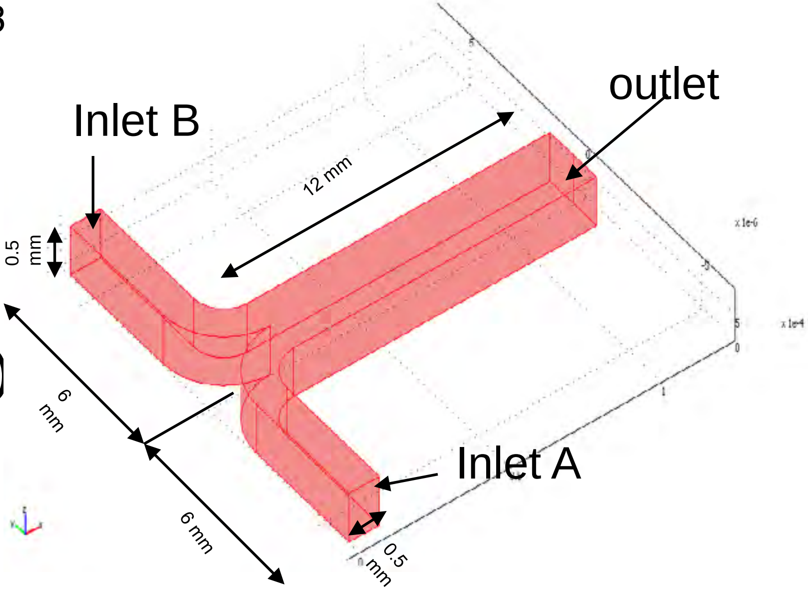
$C_{A0} = 1\ \mathrm{mol/m^3}$

$C_{B0} = 1\ \mathrm{mol/m^3}$

a = 2; b = 1; c = 2, d = 1;

n = 1; m = 2; kf = 1.5

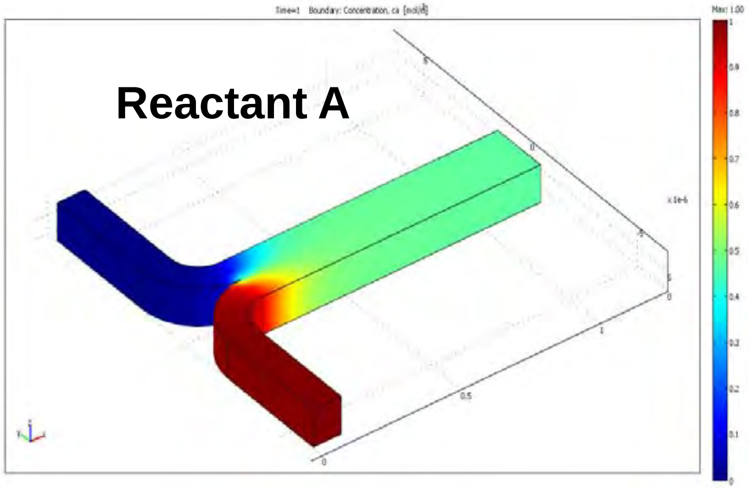
- Model Geometry (Same as T-Micromixer)



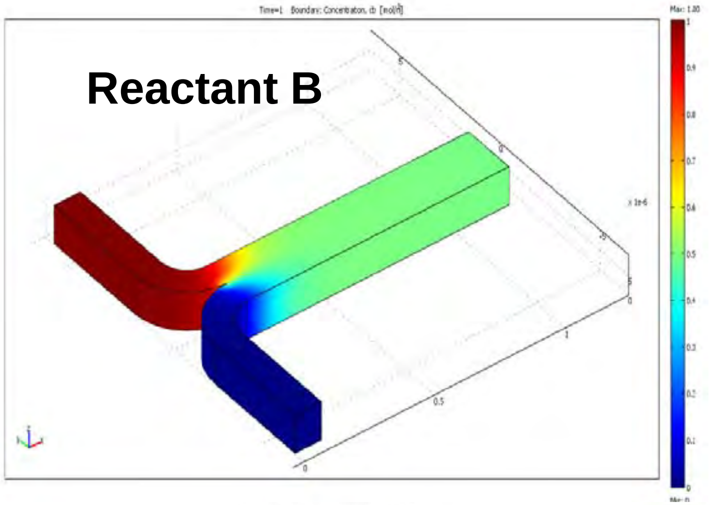
- Transport Equations for Each Specie

  - Navier-Stokes Equation for the Velocity Profiles
  - Transient Convection-Diffusion Equation for Each Specie

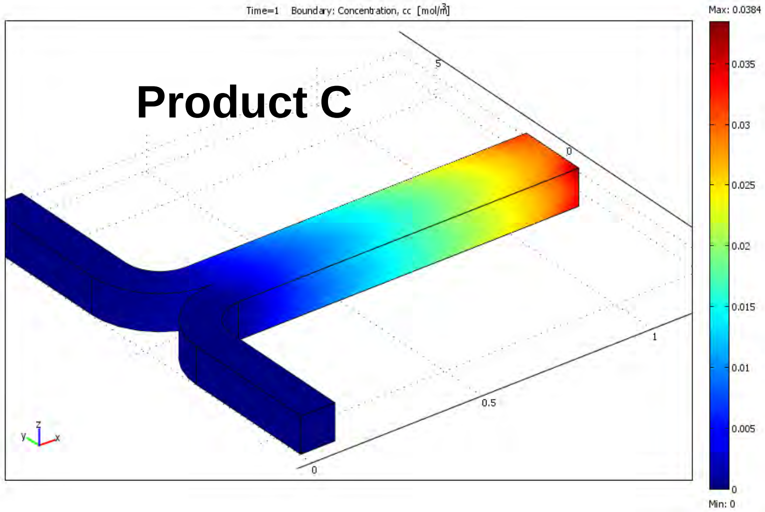
Concentration Profiles



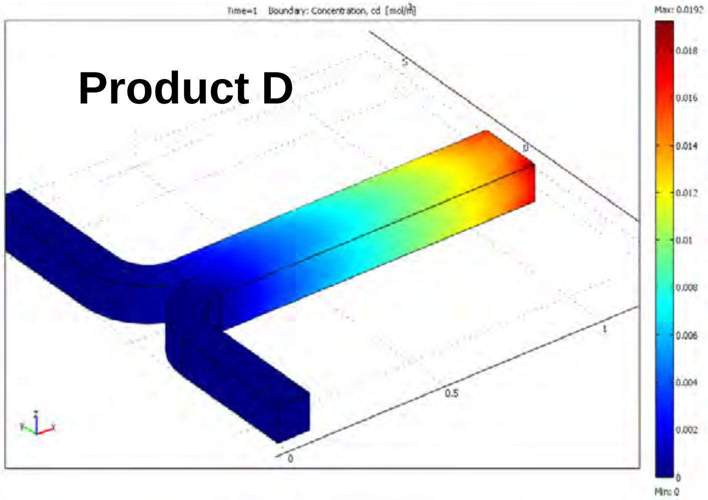
Reactant A



Reactant B



Product C



Product D

Learning Objectives

(May be Mapped to ABET Outcomes)

1. **Learned to work within budget constraints**
2. **Applied course material to real-life, open-ended project**
3. **Established connection between Chemical Engineering discipline and community, people, and values.**
4. **Learned simple project management tools**
5. **Enhanced understanding of societal impacts of engineering**
6. **Demonstrated understanding of environmental and sustainability issues in regard to water and energy conservation, and waste minimization**
7. **Identified the needs of low-income families and evaluated the importance of volunteer work**
8. **Better understood how a non-profit organization works**
9. **Extended experience in written and oral communication with a diverse audience of peers, faculty advisors, and community partners.**
10. **Learned to acquire information and knowledge independently as deemed by the project**
11. **Demonstrated ability to function in peer teams**

Future Efforts

- Development of additional examples with broader capability
- Integration of microcomponents into microprocess systems

Thank you